Introduction to structured programming with `Fortran`

https://gogs.elic.ucl.ac.be/pbarriat/learning-fortran

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Fortran : shall we start ?

- You know already one computer language ?
- You understand the very basic programming concepts :
  - What is a variable, an assignment, function call, etc.?
  - Why do I have to compile my code?
  - What is an executable?
- You (may) already know some Fortran ?
- How to proceed from old Fortran, to much more modern languages like Fortran 90/2003 ?

Why to learn Fortran ?

- Because of the execution `speed` of a program
- Well suited for numerical computations :
  more than 45% of scientific applications are in Fortran
- `Fast` code : compilers can optimize well
- Optimized `numerical libraries` available
- Fortran is a `simple` langage and it is (kind-of) `easy to learn`

Fortran is simple

- **We want to get our science done! Not learn languages!**
- How easy/difficult is it really to learn Fortran ?
- The concept is easy:
  variables, operators, controls, loops, subroutines/functions
- **Invest some time now, gain big later!**

History

FORmula **TRAN**slation

> invented 1954-8 by John Backus and his team at IBM

- FORTRAN 66 (ISO Standard 1972)
- FORTRAN 77 (1978)
- Fortran 90 (1991)
- Fortran 95 (1997)
- Fortran 2003 (2004) → `"standard" version`
- Fortran 2008 (2010)
- Fortran 2018 (11/2018)

Starting with Fortran 77

- Old Fortran provides only the absolute minimum!
- Basic features :
  data containers (integer, float, ...), arrays, basic operators, loops, I/O, subroutines and functions
- But this version has flaws:
  no dynamic memory allocation, old & obsolete constructs, “spaghetti” code, etc.
- Is that enough to write code ?

Fortran 77 → Fortran >90

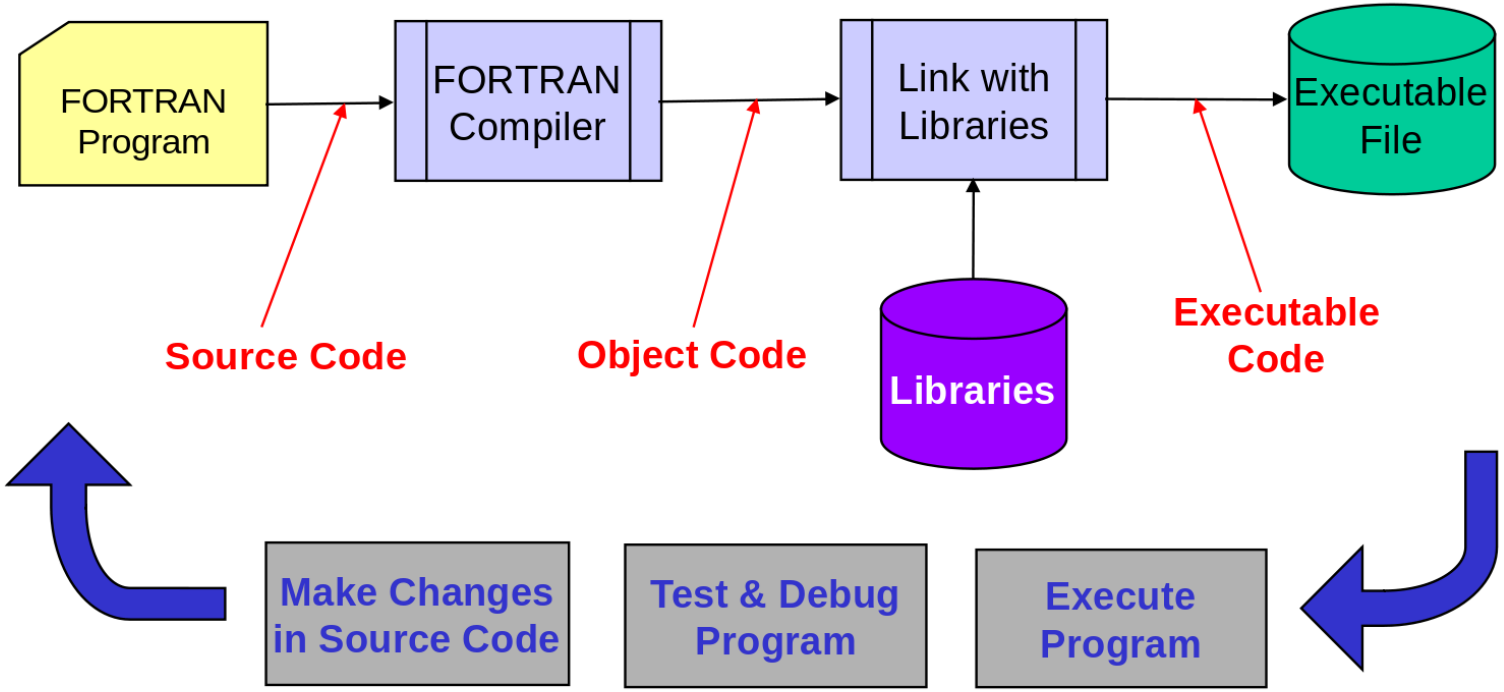
- If Fortran 77 is so simple, why is it then so difficult to write good code?
- Is simple really better?

  ⇒ Using a language allows us to express our thoughts (on a computer)
- A more sophisticated language allows for more complex thoughts
- More language elements to get organized

  ⇒ Fortran 90/95/2003 (recursive, OOP, etc)

How to Build a FORTRAN Program

FORTRAN is a compiled language (like C) so the source code (what you write) must be converted into machine code before it can be executed (e.g. Make command)



FORTRAN 77 Format

This version requires a fixed format for programs

```
      PROGRAM MAIN
C COMMENTS ARE ALLOWED IF A “C” IS PLACED IN COLUMN #1
      DIMENSION X(10)
      READ(5,*) (X(I),I=1,10)
      WRITE(6,1000) X
 1000 FORMAT(1X,’THIS IS A VERY LONG LINE OF TEXT TO SHOW HOW TO CONTINUE ’
     *  ‘THE STATEMENT TO A SECOND LINE’,/,10F12.4)
```

1-5 Label

6 (Any character: continuation line)

7-72 Statements

73-80 Optional Line #s

- max length variable names is 6 characters
- alphanumeric only, must start with a letter
- character strings are case sensitive

FORTRAN >90 Format

Versions >90 relaxe these requirements:

- comments following statements (! delimiter)
- long variable names (31 characters)
- containing only letters, digits or underscore
- max row length is 132 characters
- can be max 39 continuation lines
- if a line is ended with ampersand (&), the line continues onto the next line
- semicolon (;) as a separator between statements on a single line
- allows free field input

Program Organization

Most FORTRAN programs consist of a main program and one or more subprograms

There is a fixed order:

```
Heading
Declarations
Variable initializations
Program code
Format statements

Subprogram definitions
(functions & subroutines)
```

Data Type Declarations

Basic data types are :

- `INTEGER` : integer numbers (+/-)
- `REAL` : floating point numbers
- `DOUBLE PRECISION` : extended precision floating point
- `CHARACTER*n` : string with up to **n** characters
- `LOGICAL` : takes on values `.TRUE.` or `.FALSE.`

Data Type Declarations

`INTEGER` and `REAL` can specify number of bytes to use

- Default is: `INTEGER*4` and `REAL*4`
- `DOUBLE PRECISION` is same as `REAL*8`

Arrays of any type must be declared:

- `DIMENSION A(3,5)` - declares a 3 x 5 array
- `CHARACTER*30 NAME(50)` - directly declares a character array with 30 character strings in each element

Data Type Declarations

FORTRAN >90 allows user defined types

```
TYPE my_variable
  character(30)             :: name
  integer                   :: id
  real(8)                   :: value
  integer, dimension(3,3) :: dimIndex
END TYPE variable

type(my_variable) var
var%name = "salinity"
var%id   = 1
```

Implicit vs Explicit Declarations

By default, an implicit type is assumed depending on the first letter of the variable name:

- `A-H, O-Z` define REAL variables
- `I-N` define INTEGER variables

Can use the IMPLICIT statement:

```
IMPLICIT REAL (A-Z)
```

> makes all variables REAL if not declared

Implicit vs Explicit Declarations

```
IMPLICIT CHARACTER*2 (W)
```

> makes variables starting with W be 2-character strings

```
IMPLICIT DOUBLE PRECISION (D)
```

> makes variables starting with D be double precision

Good habit: force explicit type declarations

```
IMPLICIT NONE
```

> user must explicitly declare all variable types

Assignment Statements

Old assignment statement: `<label> <variable> = <expression>`

- `<label>` : statement label number (1 to 99999)
- `<variable>` : FORTRAN variable
  (max 6 characters, alphanumeric only for standard FORTRAN 77)

Expression:

- Numeric expressions: `VAR = 3.5*COS(THETA)`
- Character expressions: `DAY(1:3) = 'TUE'`
- Relational expressions: `FLAG = ANS .GT. 0`
- Logical expressions: `FLAG = F1 .OR. F2`

Numeric Expressions

Arithmetic operators: precedence: `**` *(high)* → `-` *(low)*

Operator	Function
`**`	exponentiation
`*`	multiplication
`/`	division
`+`	addition
`-`	subtraction

Numeric Expressions

Numeric expressions are up-cast to the highest data type in the expression according to the precedence:

(low) logical → integer → real → complex *(high)*

and smaller byte size *(low)* to larger byte size *(high)*

Example:

> fortran 77 source code arith.f

Character Expressions

Only built-in operator is **Concatenation** defined by `//`

```
'ILL'//'-'//'ADVISED'
```

`character` arrays are most commonly encountered

- treated like any array (indexed using : notation)
- fixed length (usually padded with blanks)

Character Expressions

Example:

```
CHARACTER FAMILY*16
FAMILY = ‘GEORGE P. BURDELL’

PRINT*,FAMILY(:6)
PRINT*,FAMILY(8:9)
PRINT*,FAMILY(11:)
PRINT*,FAMILY(:6)//FAMILY(10:)
```

```
GEORGE
P.
BURDELL
GEORGE BURDELL
```

Relational Expressions

Two expressions whose values are compared to determine whether the relation is true or false

- may be numeric (common) or non-numeric

`character` strings can be compared

- done character by character
- shorter string is padded with blanks for comparison

Relational Expressions

Operator	Relationship
`.LT.` or `<`	less than
`.LE.` or `<=`	less than or equal to
`.EQ.` or `==`	equal to
`.NE.` or `/=`	not equal to
`.GT.` or `>`	greater than
`.GE.` or `>=`	greater than or equal to

Logical Expressions

Consists of one or more logical operators and logical, numeric or relational operands

- values are `.TRUE.` or `.FALSE.`
- need to consider overall operator precedence

> can combine logical and integer data with logical operators but this is tricky (**avoid!**)

Logical Expressions

F77 Operator	>F90 Operator	Example	Meaning
`.AND.`	`&&`	`A .AND. B`	logical `AND`
`.OR.`	`||`	`A .OR. B`	logical `OR`
`.EQV.`	`==`	`A .EQV. B`	logical equivalence
`.NEQV.`	`/=`	`A .NEQV. B`	logical inequivalence
`.XOR.`	`/=`	`A .XOR. B`	exclusive `OR` (same as `.NEQV.`)
`.NOT.`	`!`	`.NOT. A`	logical negation

Arrays in FORTRAN

Arrays can be multi-dimensional (up to 7 in F77) and are indexed using `( )`:

- `TEST(3)` or `FORCE(4,2)`

> Indices are by default defined as `1...N`

We can specify index range in declaration

- `INTEGER K(0:11)` : `K` is dimensioned from `0-11` (12 elements)

Arrays are stored in column order (1st column, 2nd column, etc) so accessing by incrementing row index first usually is fastest

Whole array reference (only in >F90): `K(:)=-8` assigns 8 to all elements in K

> Avoid `K=-8` assignement

Unconditional `GO TO` in F77

This is the only GOTO in FORTRAN 77

- Syntax: `GO TO label`
- Unconditional transfer to labeled statement

```
10   -code-
     GO TO 30
     -code that is bypassed-
30   -code that is target of GOTO-
     -more code-
     GO TO 10
```

- **Problem** : leads to confusing *"spaghetti code"* 💥

`IF ELSE IF` Statement

Basic version:

```
IF (KSTAT.EQ.1) THEN
  CLASS='FRESHMAN'
ELSE IF (KSTAT.EQ.2) THEN
  CLASS='SOPHOMORE'
ELSE IF (KSTAT.EQ.3) THEN
  CLASS='JUNIOR'
ELSE IF (KSTAT.EQ.4) THEN
  CLASS='SENIOR'
ELSE
  CLASS='UNKNOWN'
ENDIF
```

Spaghetti Code in F77 (and before)

Use of `GO TO` and arithmetic `IF`'s leads to bad code that is very hard to maintain

Here is the equivalent of an `IF-THEN-ELSE` statement:

```
10  IF (KEY.LT.0) GO TO 20
    TEST=TEST-1
    THETA=ATAN(X,Y)
    GO TO 30
20  TEST=TEST+1
    THETA=ATAN(-X,Y)
30  CONTINUE
```

Now try to figure out what a complex `IF ELSE IF` statement would look like coded with this kind of simple `IF`...

Loop Statements (old versions)

`DO` loop: structure that executes a specified number of times

Spaghetti Code Version

```
      K=2
 10   PRINT*,A(K)
      K=K+2
      IF (K.LE.11) GO TO 10
 20   CONTINUE
```

F77 Version

```
      DO 100 K=2,10,2
      PRINT*,A(K)
100   CONTINUE
```

Loop Statements (>F90)

```
DO K=2,10,2
  WRITE(*,*) A(K)
END DO
```

- Loop _control can include variables and a third parameter to specify increments, including negative values
- Loop always executes ONCE before testing for end condition

```
READ(*,*) R
DO WHILE (R.GE.0)
  VOL=2*PI*R**2*CLEN
  READ(*,*) R
END DO
```

- Loop will not execute at all if logical_expr is not true at start

Comments on Loop Statements

In old versions:

- to transfer out (exit loop), use a `GO TO`
- to skip to next loop, use `GO TO` terminating statement (this is a good reason to always make this a `CONTINUE` statement)

In new versions:

- to transfer out (exit loop), use `EXIT` statement and control is transferred to statement following loop end. This means you cannot transfer out of multiple nested loops with a single `EXIT` statement (use named loops if needed - `myloop : do i=1,n`). This is much like a `BREAK` statement in other languages.
- to skip to next loop cycle, use `CYCLE` statement in loop.

File-Directed Input and Output

Much of early FORTRAN was devoted to reading input data
from Cards and writing to a line printer

Today, most I/O is to and from a file: it requires more extensive I/O capabilities standardized until FORTRAN 77

I/O = communication between a program and the outside world

- opening and closing a file with `OPEN` & `CLOSE`
- data reading & writing with `READ` & `WRITE`
- can use **unformatted** `READ` & `WRITE` if no human readable data are involved (much faster access, smaller files)

OPEN & CLOSE example

Once opened, file is referred to by an assigned device number (a unique id)

```
character(len=*) :: x_name
integer          :: ierr, iSize, guess_unit
logical          :: itsopen, itexists
!
inquire(file=trim(x_name), size=iSize, number=guess_unit, opened=itsopen, exist=itexists)
if ( itsopen ) close(guess_unit, status='delete')
!
open(902,file=trim(x_name),status='new',iostat=ierr)
!
if (iSize <= 0 .OR. .NOT.itexists) then
  open(902,file=trim(x_name),status='new',iostat=ierr)
  if (ierr /= 0) then
    ...
    close(902)
  endif
  ...
endif
```

`READ` Statement

- syntax: `READ(dev_no, format_label) variable_list`
- read a record from `dev_no` using `format_label` and assign results to variables in `variable_list`

```
      READ(105,1000) A,B,C
1000  FORMAT(3F12.4)
```

> device numbers 1-7 are defined as standard I/O devices

- each `READ` reads one or more lines of data and any remaining data in a line that is read is dropped if not translated to one of the variables in the `variable_list`
- `variable_list` can include implied `DO` such as: `READ(105,1000)(A(I),I=1,10)`

`READ` Statement - cont'd

- input items can be integer, real or character
- characters must be enclosed in `' '`
- input items are separated by commas
- input items must agree in type with variables in `variable_list`
- each `READ` processes a new record (line)

```
INTEGER K
REAL(8) A,B
OPEN(105,FILE='path_to_existing_file')
READ(105,*) A,B,K
```

> read one line and look for floating point values for A and B and an integer for K

`WRITE` Statement

- syntax: `WRITE(dev_no, format_label) variable_list`
- write variables in `variable_list` to output `dev_no` using format specified in format statement with `format_label`

```
      WRITE(*,1000) A,B,KEY
 1000 FORMAT(F12.4,E14.5,I6)
```

```
|----+----o----+----o----+----o----+----|
    1234.5678  -0.12345E+02     12
```

- device number `*` is by default the screen (or *standard output* - also 6)
- each `WRITE` produces one or more output lines as needed to write out `variable_list` using `format` statement
- `variable_list` can include implied `DO` such as: `WRITE(*,2000)(A(I),I=1,10)`

`FORMAT` Statement

data type	format descriptors	example
`integer`	`iw`	`write(*,'(i5)') int`
`real` (*decimal*)	`fw.d`	`write(*,'(f7.4)') x`
`real` (*exponential*)	`ew.d`	`write(*,'(e12.3)') y`
`character`	`a, aw`	`write(*,'(a)') string`
`logical`	`lw`	`write(*,'(l2)') test`
spaces & tabs	`wx` & `tw`	`write (*,'(i3,2x,f6.3)') i, x`
linebreak	`/`	`write (*,'(f6.3,/,f6.3)') x, y`

NAMELIST

It is possible to pre-define the structure of input and output data using `NAMELIST` in order to make it easier to process with `READ` and `WRITE` statements

- Use `NAMELIST` to define the data structure
- Use `READ` or `WRITE` with reference to `NAMELIST` to handle the data in the specified format

> This is not part of standard F77 but it is included in >F90

On input, the `NAMELIST` data must be structured as follows:

```
&INPUT
  THICK=0.245,
  LENGTH=12.34,
  WIDTH=2.34,
  DENSITY=0.0034
/
```

Internal `WRITE` Statement

Internal `WRITE` does same as `ENCODE` in F77 : **a cast to string**

> `WRITE (dev_no, format_label) var_list`
>
> write variables in `var_list` to internal storage defined by character variable used as `dev_no` = default character variable (not an array)

```
INTEGER*4 J,K
CHARACTER*50 CHAR50
DATA J,K/1,2/
...
WRITE(CHAR50,*) J,K
```

Results:

```
CHAR50='    1      2'
```

Internal `READ` Statement

Internal `READ` does same as `DECODE` in F77 : **a cast from string**

> `READ (dev_no, format_label) var_list`
>
> read variables from internal storage specified by character variable used as
>
> `dev_no` = default character variable (not an array)

```
INTEGER K
REAL A,B
CHARACTER*80 REC80
DATA REC80/'1.2, 2.3, -5'/
...
READ(REC80,*) A,B,K
```

Results:

```
A=1.2, B=2.3, K=-5
```

Structured programming

Structured programming is based on subprograms (functions and subroutines) and control statements (like `IF` statements or loops) :

- structure the control-flow of your programs (eg, give up the `GO TO`)
- improved readability
- lower level aspect of coding in a smart way

It is a **programming paradigm** aimed at improving the quality, clarity, and access time of a computer program

Functions and Subroutines

`FUNCTION` & `SUBROUTINE` are subprograms that allow structured coding

- `FUNCTION`: returns a single explicit function value for given function arguments
  It's also a variable → so must be declared !
- `SUBROUTINE`: any values returned must be returned through the arguments (no explicit subroutine value is returned)
- functions and subroutines are **not recursive in F77**

Subprograms use a separate namespace for each subprogram so that variables are local to the subprogram

- variables are passed to subprogram through argument list and returned in function value or through arguments
- variables stored in `COMMON` may be shared between namespaces

Functions and Subroutines - cont'd

Subprograms must include at least one `RETURN` (can have more) and be terminated by an `END` statement

`FUNCTION` example:

```
REAL FUNCTION AVG3(A,B,C)
AVG3=(A+B+C)/3
RETURN
END
```

Use:

```
AV = WEIGHT*AVG3(A1,F2,B2)
```

> `FUNCTION` type is implicitly defined as REAL

Functions and Subroutines - cont'd

Subroutine is invoked using the `CALL` statement

`SUBROUTINE` example:

```
SUBROUTINE AVG3S(A,B,C,AVERAGE)
AVERAGE=(A+B+C)/3
RETURN
END
```

Use:

```
CALL AVG3S(A1,F2,B2,AVR)
RESULT = WEIGHT*AVR
```

> any returned values must be returned through argument list

Arguments

Arguments in subprogram are `dummy` arguments used in place of the real arguments

- arguments are passed by **reference** (memory address) if given as *symbolic*
  the subprogram can then alter the actual argument value since it can access it by reference
- arguments are passed by **value** if given as *literal* (so cannot be modified)

```
CALL AVG3S(A1,3.4,C1,QAV)
```

> 2nd argument is passed by value - QAV contains result

```
CALL AVG3S(A,C,B,4.1)
```

> no return value is available since "4.1" is a value and not a reference to a variable!

Arguments - cont'd

- `dummy` arguments appearing in a subprogram declaration cannot be an individual array element reference, e.g., `A(2)`, or a *literal*, for obvious reasons!
- arguments used in invocation (by calling program) may be *variables*, *subscripted variables*, *array names*, *literals*, *expressions* or *function names*
- using symbolic arguments (variables or array names) is the **only way** to return a value (result) from a `SUBROUTINE`

> It is considered **BAD coding practice**, but functions can return values by changing the value of arguments
> This type of use should be strictly **avoided**!

Arguments - cont'd

The `INTENT` keyword (>F90) increases readability and enables better compile-time error checking

```
SUBROUTINE AVG3S(A,B,C,AVERAGE)
  IMPLICIT NONE
  REAL, INTENT(IN)    :: A, B
  REAL, INTENT(INOUT) :: C             ! default
  REAL, INTENT(OUT)   :: AVERAGE

  A = 10                               ! Compilation error
  C = 10                               ! Correct
  AVERAGE=(A+B+C)/3                    ! Correct
END
```

> Compiler uses `INTENT` for error checking and optimization

`FUNCTION` versus Array

`REMAINDER(4,3)` could be a 2D array or it could be a reference to a function

If the name, including arguments, **matches an array declaration**, then it is taken to be an array, **otherwise**, it is assumed to be a `FUNCTION`

Be careful about `implicit` versus `explicit` type declarations with `FUNCTION`

```
PROGRAM MAIN
  INTEGER REMAINDER
  ...
  KR = REMAINDER(4,3)
  ...
END

INTEGER FUNCTION REMAINDER(INUM,IDEN)
  ...
END
```

Arrays with Subprograms

Arrays present special problems in subprograms

- must pass by reference to subprogram since there is no way to list array values explicitly as literals
- how do you tell subprogram how large the array is ?

> Answer varies with FORTRAN version and vendor (dialect)...

When an array element, e.g. `A(1)`, is used in a subprogram invocation (in calling program), it is passed as a reference (address), just like a simple variable

When an array is used by name in a subprogram invocation (in calling program), it is passed as a reference to the entire array. In this case the array must be appropriately dimensioned in the subroutine (and this can be tricky...)

Arrays - cont'd

Data layout in multi-dimensional arrays

- always increment the left-most index of multi-dimensional arrays in the innermost loop (i.e. fastest)
- **column major** ordering in Fortran vs. **row major** ordering in C
- a compiler (with sufficient optimization flags) may re-order loops automatically

```
do j=1,M
  do i=1,N ! innermost loop
    y(i) = y(i)+ a(i,j)*x(j) ! left-most index is i
  end do
end do
```

Arrays - cont'd

- dynamically allocate memory for arrays using `ALLOCATABLE` on declaration
- memory is allocated through `ALLOCATE` statement in the code and is deallocated through `DEALLOCATE` statement

```
integer :: m, n
integer, allocatable :: idx(:)
real, allocatable :: mat(:,:)
m = 100 ; n = 200
allocate( idx(0:m-1))
allocate( mat(m, n))
...
deallocate(idx , mat)
```

> It exists many array intrinsic functions: SIZE, SHAPE, SUM, ANY, MINVAL, MAXLOC, RESHAPE, DOT_PRODUCT, TRANSPOSE, WHERE, FORALL, etc

`COMMON` & `MODULE` Statement

The `COMMON` statement allows variables to have a more extensive scope than otherwise

- a variable declared in a `Main Program` can be made accessible to subprograms (without appearing in argument lists of a calling statement)
- this can be selective (don't have to share all everywhere)
- **placement**: among type declarations, after `IMPLICIT` or `EXPLICIT`, before `DATA` statements
- can group into **labeled** `COMMON`

With > F90, it's better to use the `MODULE` subprogram instead of the `COMMON` statement

Modular programming (>F90)

Modular programming is about separating parts of programs into independent and interchangeable modules :

- improve testability
- improve maintainability
- re-use of code
- higher level aspect of coding in a smart way
- *separation of concerns*

The principle is that making significant parts of the code independent, replaceable and independently testable makes your programs **more maintainable**

Subprograms type

`MODULE` are subprograms that allow modular coding and data encapsulation

The interface of a subprogram type is **explicit** or **implicit**

Several types of subprograms:

- `intrinsic`: explicit - defined by Fortran itself (trignonometric functions, etc)
- `module`: explicit - defined with `MODULE` statement and used with `USE`
- `internal`: explicit - defined with `CONTAINS` statement inside (sub)programs
- `external`: implicit (but can be manually (re)defined explicit) - e.g. **libraries**

Differ with the **scope**: what data and other subprograms a subprogram can access

MODULE type

```
MODULE example
  IMPLICIT NONE
  INTEGER, PARAMETER :: index = 10
  REAL(8), SAVE      :: latitude
CONTAINS
  FUNCTION check(x) RESULT(z)
  INTEGER :: x, z
  ...
  END FUNCTION check
END MODULE example
```

```
PROGRAM myprog
  USE example, ONLY: check, latitude
  IMPLICIT NONE
  ...
  test = check(a)
  ...
END PROGRAM myprog
```

`internal` subprogams

```fortran
program main
  implicit none
  integer N
  real X(20)
  ...
  write(*,*), 'Processing x...', process()
  ...
contains
  logical function process()
    ! in this function N and X can be accessed directly (scope of main)
    ! Please not that this method is not recommended:
    ! it would be better to pass X as an argument of process
    implicit none
    if (sum(x) > 5.) then
       process = .FALSE.
    else
       process = .TRUE.
    endif
  end function process
end program
```

`external` subprogams

- `external` subprogams are defined in a separate program unit
- to use them in another program unit, refer with the `EXTERNAL` statement
- compiled separately and linked

!!! DO NOT USE THEM: modules are much easier and more robust ❗

They are only needed when subprogams are written with different programming language or when using external libraries (such as BLAS)

> It's **highly** recommended to construct `INTERFACE` blocks for any external subprogams used

`interface` statement

```
SUBROUTINE nag_rand(table)
  INTERFACE
    SUBROUTINE g05faf(a,b,n,x)
      REAL, INTENT(IN)    :: a, b
      INTEGER, INTENT(IN) :: n
      REAL, INTENT(OUT)   :: x(n)
    END SUBROUTINE g05faf
  END INTERFACE
  !
  REAL, DIMENSION(:), INTENT(OUT) :: table
  !
  call g05faf(-1.0,-1.0, SIZE(table), table)
END SUBROUTINE nag_rand
```

Conclusions

- Fortran in all its standard versions and vendor-specific dialects is a rich but confusing language
- Fortran is a modern language that continues to evolve
- Fortran is still ideally suited for numerical computations in engineering and science
  - most new language features have been added since F95
  - "High Performance Fortran" includes capabilities designed for parallel processing